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α-Al_2O_3(0001)-(1×1) surface structure

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The structure, composition and morphology of ceramic surfaces strongly influence their chemical, mechanical and electrical properties and thus have a dominant contribution in many technologically important processes such as corrosion, catalysis and sintering. They also affect the nature and strength of bonding at metal/ceramic interfaces used in composites or in electronic packaging. The (0001) surface of a-alumina is of major importance : it is one of the most widely used substrate for thin film growth and its initial state is known to play a dominant role on the overlayer properties. Despite this interest, little is known about the structure and energetics of oxide surfaces. In particular, the nature of the terminating plane (Al or 0) and the relaxations of the α-Al_2O_3(0001) unreconstructed surface was still an open topic, theoretical calculations yielding different answers.

We have experimentally determined these parameters for the first time by a Grazing Incidence X-ray Scattering (GIXS) study using the ID03 surface diffraction setup. This surface of very light material could only be studied with a high brillance undulator beam such as the one of ID03. It allowed to avoid the large background intensity coming from1 bulk defect by using 10 μm slits perpendicular to the surface, at a very grazing incident angle of 0.1°, enabling measurements of very weak Crystal Truncation Rods (CTRs) in between Bragg peaks.

By using a high beam energy, (7"' harmonic at 23 keV), about 900 non-equivalent CTRs points were collected, up to large perpendicular momentum transfer of 7 $Å^{-1}$ (Fig. 1). Least-square fitting was performed in order to determine the chemical termination (0 plane, single Al plane or double Al plane) and surface relaxations. Fig. 1 shows clearly that the 0 termination can be ruled out : a good fit of the (10 ℓ) rod cannot be achieved with this model, even with large atomic displacements. Single and double Al terminations yield very similar χ^2 values. However, the latter yields an outward relaxation of the outermost Al plane of +93 %, which is very unlikely. Moreover, for this model, the "bump" at ℓ ~ -3.5 on the (10 ℓ) rod is not reproduced.

The most likely surface is therefore terminated with a single Al plane. This agrees with most theoretical results, based on the fact that there must be no net dipole moment at the surface. This is also the only termination which leaves the surface "autocompensated", i.e. both charge neutral and chemically stable.

Regarding the surface relaxations (Fig. 2), theoretical results differ depending on the method used. However they all agree with a large negative relaxation of the topmost Al layer, which is also our conclusion, the first interplanar spacing being reduced by -51%. However, the first Al-0 bond length is only 4.5% shorter than the bulk one because the underlying oxygen atoms shift mainly parallel to the surface plane as they are repelled from the top Al atoms, moving almost radially towards the second Al sites. This almost bond length conservative relaxation has also been theoretically predicted.

Publication : Applications of Synchrotron Radiation to Materials Science III", Mat. Res. Soc. Symp. Proc, Vol. 437, p15-20 (1996).

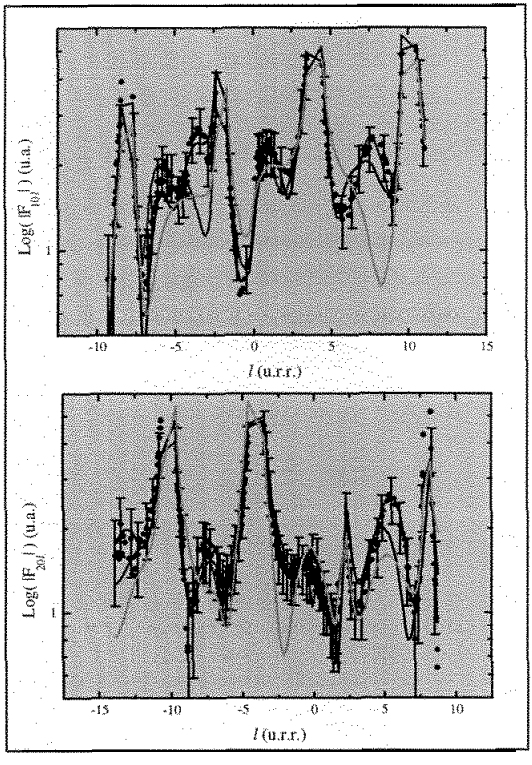

Fig. 1 : (10*l*) and (20*l*) structure factors : experimental data (blue) and best fits for 0 (green). double Al (black) and Al (red) terminations.

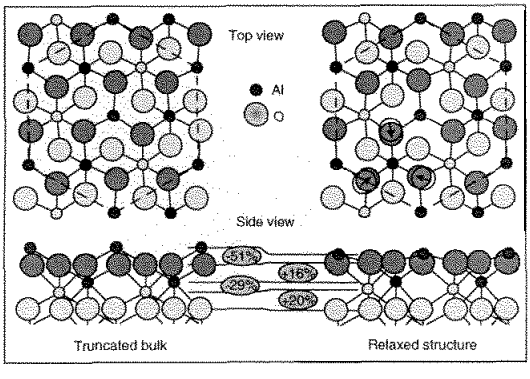

Fig. 2 : Model deduced from the best fit : Top and side views of the 5 first atomic planes of the α-Al_2O_3(0001) surface